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Exactly massless quarks on the lattice.

Herbert Neuberger

*Department of Physics and Astronomy
Rutgers University
Piscataway, NJ 08855-0849*

Abstract

It is suggested that the fermion determinant for a vector-like gauge theory with strictly massless quarks can be represented on the lattice as $\det \frac{1+V}{2}$, where $V = X(X^\dagger X)^{-1/2}$ and X is the Wilson-Dirac lattice operator with a negative mass term. There is no undesired doubling and no need for any fine tuning. Several other appealing features of the formula are pointed out.

From the start, it was awkward to ensure masslessness of quarks in lattice QCD. Without masslessness there are no chiral symmetries and no massless pions. Massless QCD is a beautiful parameter free theory in the continuum, just like pure YM is. However, while pure YM on the lattice is elegant, the addition of quarks makes the lattice theory less appealing. The overlap [1, 2, 3] provided a solution to this state of affairs; however, the formalism is a bit complicated, and its elegance becomes a matter of personal taste. More importantly, the computational cost seems to be daunting. Domain walls [4, 5, 6] provide an approximation to the overlap, but they sacrifice strict masslessness, so we are back to the more murky situation of standard formulations. Staggered fermions do preserve masslessness, but it is a nuisance to have so many of them, and the connection to continuum operators is messy. My purpose here is to present a simple formula for the fermion determinant which I argue is equivalent to the overlap but is much more attractive in appearance. Only future work can tell with any confidence whether real practical progress has been made, but there are some very attractive features that I wish to point out.

The basic observation stems from recent work [7] on the overlap in odd dimensions. For $d = 2k + 1$ the overlap for Dirac fermions can be written as the determinant of a finite matrix of fixed shape. This simpler formula descends by dimensional reduction from $d + 1$ dimensions where it represented Weyl fermions in a less explicit formulation. Dimensionally reducing again, a simple formula for Dirac fermions in $2k$ dimensions is obtained. To make this letter relatively self-contained, I present a more direct derivation, involving no dimensional reductions.

In [1] the overlap for a vector-like theory is constructed as follows: The chiral determinant is replaced at the regulated level by the overlap of two many-body states. These are the ground states of two bilinear Hamiltonians,

$$\mathcal{H}^\pm = a^\dagger H^\pm a, \tag{1}$$

with all indices suppressed. The matrices H^\pm are obtained from

$$H(m) = \begin{pmatrix} B + m & C \\ C^\dagger & -B - m \end{pmatrix} \tag{2}$$

with $H^+ = H(\infty)$, $H^- = H(-m_0)$ and $0 < m_0 < 2$. The infinite argument for H^+ can be replaced by any finite positive number, but the equations are somewhat simpler with our

choice [8, 9, 10]. The matrices C and B are given below:

$$\begin{aligned} (C)_{x\alpha i, y\beta j} &= \frac{1}{2} \sum_{\mu=1}^{2k} \sigma_{\mu}^{\alpha\beta} [\delta_{y, x+\hat{\mu}} (U_{\mu}(x))_{ij} - \delta_{x, y+\hat{\mu}} (U_{\mu}^{\dagger}(y))_{ij}], \\ (B)_{x\alpha i, y\beta j} &= \frac{1}{2} \delta_{\alpha\beta} \sum_{\mu=1}^{2k} [2\delta_{xy} \delta_{ij} - \delta_{y, x+\hat{\mu}} (U_{\mu}(x))_{ij} - \delta_{x, y+\hat{\mu}} (U_{\mu}^{\dagger}(y))_{ij}]. \end{aligned} \quad (3)$$

x, y are sites on the lattice, α, β are Weyl spinor indices and i, j are color indices. The σ_{μ} are Euclidean Weyl matrices in $2k$ dimensions. The overlap O , is given by

$$O = | \langle v_+ | v_- \rangle |^2, \quad \mathcal{H}^{\pm} |v_{\pm}\rangle = E_{\min}^{\pm} |v_{\pm}\rangle. \quad (4)$$

An equivalent representation is also given in [1]:

$$O = | \langle v_+ | v_- \rangle | | \langle t_+ | t_- \rangle |, \quad \mathcal{H}^{\pm} |t_{\pm}\rangle = E_{\max}^{\pm} |t_{\pm}\rangle. \quad (5)$$

$E_{\min(\max)}^{\pm}$ denote minimal (maximal) energies which define the associated states, assuming no degeneracies.

I now replace the two sets of fermion operators, one for each factor in equation (5), by a single set of double their size:

$$\mathcal{H}_2^{\pm} = A^{\dagger} H_2^{\pm} A, \quad H_2^{\pm} = \begin{pmatrix} 0 & H^{\pm} \\ H^{\pm} & 0 \end{pmatrix}. \quad (6)$$

Clearly,

$$O = | \langle V_+ | V_- \rangle |, \quad \mathcal{H}_2^{\pm} |V_{\pm}\rangle = E_{\min}^{\pm} |V_{\pm}\rangle. \quad (7)$$

But, using [1] again, we immediately can write down the overlap as

$$O = | \det \frac{1 + \Gamma_{2k+1} \epsilon(H^-)}{2} |, \quad \Gamma_{2k+1} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \epsilon(H) \equiv \frac{H}{\sqrt{H^2}}, \quad (8)$$

where we assume $\det H \neq 0$ (this is equivalent to the absence of degeneracies mentioned after equation (5) above). The matrix

$$V = \Gamma_{2k+1} \epsilon(H^-) \quad (\Gamma_{2k+1}^2 = 1, \epsilon(H^-)^2 = 1) \quad (9)$$

is unitary while both factors are hermitian. Actually, the absolute sign in eq. (8) is not needed:

$$\det(1 + V) = \prod_{r=1}^{R_0} (1 + \lambda_r) \prod_{c=1}^{C_0} |1 + \lambda_c|^2 \geq 0. \quad (10)$$

Here, $\lambda_r = \lambda_r^*$ and $\lambda_c \neq \lambda_c^*$. Equation (8), without the absolute value signs, is the main result of this letter. Noting that

$$\Gamma_{2k+1} H(m) \equiv X(m) = \begin{pmatrix} B+m & C \\ -C^\dagger & B+m \end{pmatrix}, \quad (11)$$

and that

$$\begin{pmatrix} 0 & \sigma_\mu \\ \sigma_\mu^\dagger & 0 \end{pmatrix} = \gamma_\mu, \quad (12)$$

where the γ_μ are Euclidean Dirac matrices, we obtain the result announced in the abstract. $X(m)$ is the familiar Wilson Dirac operator, and we denote $X(-m_0)$ by X .

The inverse of the matrix whose determinant we have to take is easily seen to have only a single massless Dirac particle pole, so there is no unnecessary doubling [7]. In some sense our formula is a realization of an idea of Rebbi's [11], only some of the ingredients are different and there is a body of overlap work to rely on [1, 2, 3, 12].

One of the most salient properties of strictly massless fermions are the exact and robust zeros in instanton backgrounds. From the equivalence to the overlap we know that V should have -1 as an eigenvalue with degeneracy $\frac{1}{2}|\text{tr}\epsilon(H^-)|$ (the overlap lattice topological charge is given by $n_{\text{top}} = \frac{1}{2}\text{tr}\epsilon(H^-)$) and that this property is robust under small variations of the background. It is amusing to see this directly in the particular case of a single instanton or anti-instanton, where $|n_{\text{top}}| = 1$. The following identities are easily established:

$$\det(1 + V) = \det(1 + V^{-1}) = \frac{\det(1 + V)}{\det V} = \det(V) \det(1 + V). \quad (13)$$

If the number of sites is Ω , the dimension of V is $N \equiv R_0 + 2C_0 = 2^k d_R \Omega$, where d_R is the range of group indices. Clearly, N is even.

$$\det(V) = \det(\Gamma_{2k+1}) \det(\epsilon(H^-)) = (-)^{\frac{N}{2}} (-)^{\frac{N}{2} + n_{\text{top}}} = -1 \quad (14)$$

Inserting $\det(V) = -1$ into equation (13) gives $\det(1 + V) = 0$, the expected result.

Once we are willing to interpret $\frac{1+V}{2}$ as the Dirac operator, many applications in four dimensions suggest themselves. In the continuum, the spectral density of the massless Dirac operator per unit four-volume is supposed to concentrate at the origin to reproduce the chiral symmetry order parameter [13]. Attempts to show this on the lattice in the past were hindered by the eigenvalues not falling on a line in the complex plane, and it was difficult, in finite volumes, to identify and remove the effects of global topological charge, which is something one should do. Now it would be easy: all the eigenvalues of V reside

on the unit circle. Those strictly at -1 reflect global topology. Those close to -1 , but not exactly at -1 , should build up the condensate $\langle \bar{\psi}\psi \rangle$.

A related application is the measurement of f_π using a finite-size soft-pion theorem as in [14]. Since chiral symmetry is exact we do not have to deal with the more complex situation created by the presence of an explicit symmetry breaking parameter. Anyhow, the interpretation of the transition obtained by tuning the mass parameter in ordinary Wilson-Dirac formulations, while away from the continuum limit, is likely different from a full restoration of chiral symmetries as first pointed out by Aoki [15]. Therefore, working with ordinary Wilson fermions and obtaining f_π via finite size theorems is promising to be messy.

Since the eigenvalue distribution of V has the potential of behaving smoothly on the lattice there is a chance to make some progress on the painful problem of QCD at finite chemical potential [16], at least in the rather interesting situation of strictly massless quarks.

In addition to the overlap, several proposals to regulate *chiral* gauge theories maintain exact gauge invariance of the absolute value of the chiral determinant [17,18]. It is typically proposed [17] to take a square root of $|\det(X)|$ with a mass parameter finely tuned to Wilson-Aoki criticality. Clearly, this is not very appealing, since $\det(X)$ changes sign frequently in that vicinity (it is real) and the absolute value will give trouble when variations with respect to the background fields are taken, for example for the purpose of deriving a Ward identity. However, using $\sqrt{\det \frac{1+V}{2}}$ avoids this problem and is identical to the absolute value of the chiral determinant in the overlap; as a bonus the exact zeros induced by nontrivial global topology are also maintained. Maybe there is a possibility to unify in this way several different approaches to the problem of regularizing chiral gauge theories.

In recent work [19], it was shown that the method of [1] for using the overlap to count instantons gives results in perfect agreement with very different methods [20], thus providing much support for both results. By varying m_0 in the interval $(0, 2)$ a flow of V -eigenvalues on the unit circle would be induced. The eigenvalue motions on the unit circle have the potential of providing a pictorial insight via a scale-dependent (the scale is $\sim \frac{1}{m_0}$) fermionic probe of the gauge background.

Much of what I said needs further study. Some of the needed future work is analytical: With the new formulae, perturbation theory may be more compact and more Feynman-like. Of course, one needs to check whether the natural guess $\frac{2}{1+V}$ is indeed an appropriate definition of the fermion propagator, and how it is related to the continuum. Numerical work in two dimensions could check the flow patterns and see whether they are interesting.

Also, comparisons between the pure overlap and its domain wall approximations [21] might be facilitated by the new version of the formula. And, most importantly, it is an attractive, if difficult, challenge to develop an efficient numerical technique to include $\det \frac{1+V}{2}$ in dynamical simulations in four dimensions, or even to compute just the inverse $\frac{2}{1+V}$. While the problem looks hard, it does seem somewhat easier than when looking at the older form of the overlap in equation (4).

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